Projective Space Method for Slow Invariant Manifolds of Reactive Systems

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Introduction

Motivation and background

- Detailed kinetics are essential for accurate modeling of real systems.

- Reactive flow systems admit multi-scale solutions.

- Manifold methods provide a potential for computational saving.

- Slow invariant manifolds (SIMs) describe the asymptotic structure of reactive systems' invariant attracting trajectories.

- Current manifold construction methods either approximate the actual SIMs or require a close initial guess.

Long-term objective

Create an efficient algorithm that reduces the computational cost for simulating reactive flows based on a reduction in the stiffness and dimension of the composition phase space.
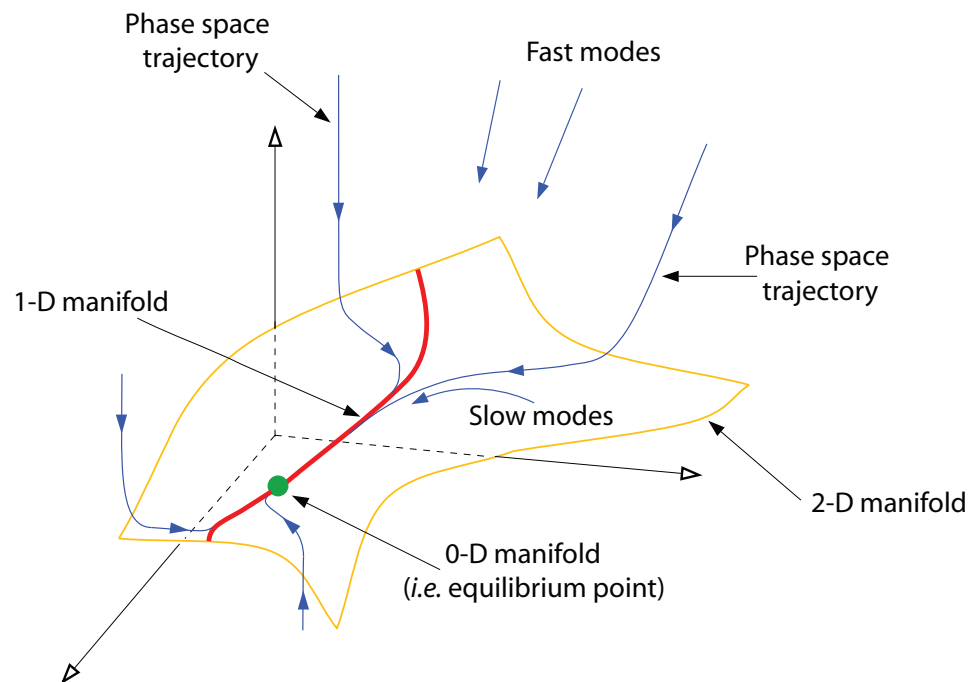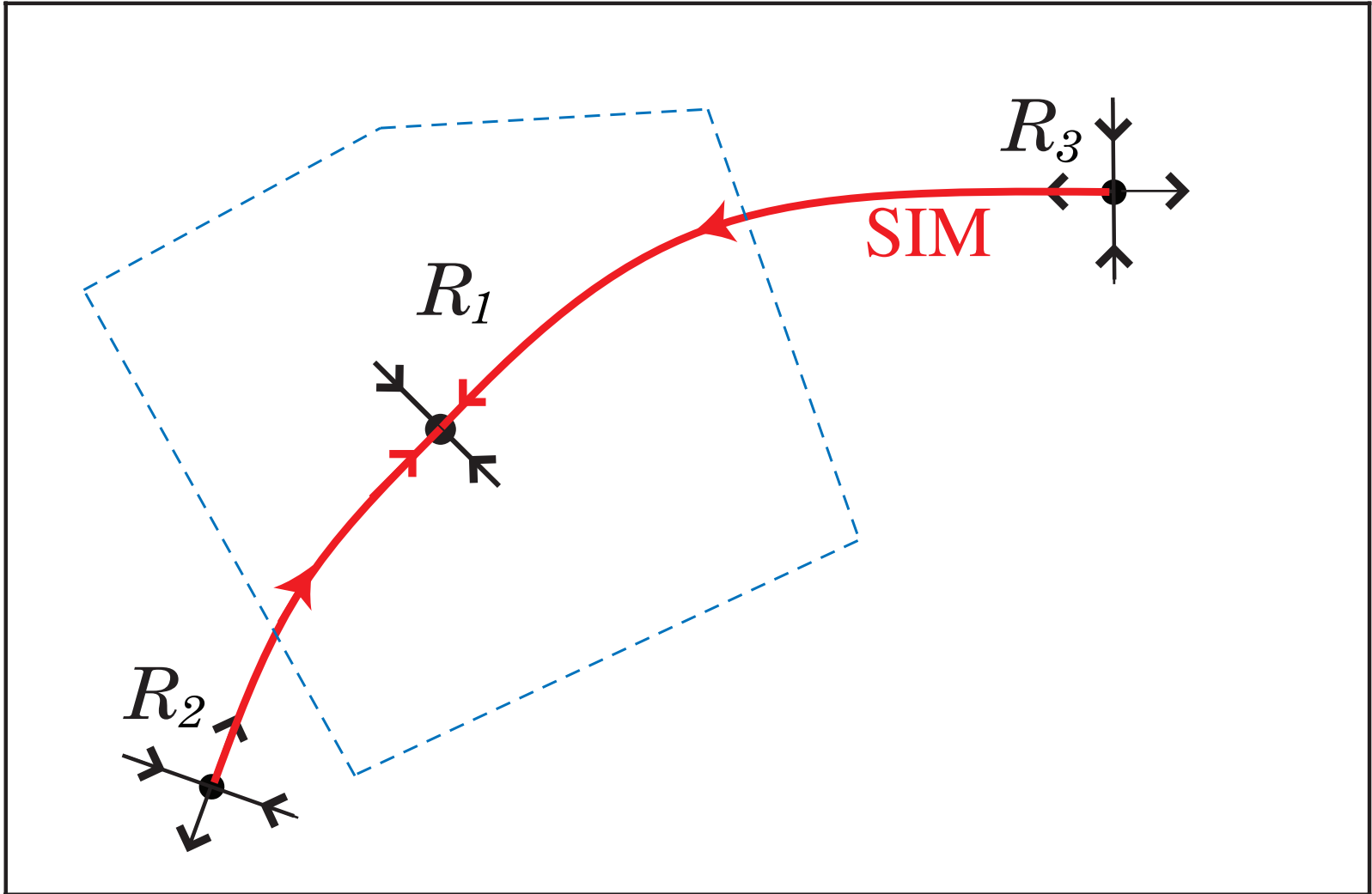

Immediate objective

Construct 1-D SIMs for dynamical systems arising from modeling unsteady spatially homogenous closed reactive systems.

Slow Invariant Manifold (SIM)

• The composition phase space for closed spatially homogeneous reactive system:

$$\frac{d\mathbf{z}}{dt} = \mathbf{f}\left(\mathbf{z}\right), \quad \mathbf{z} \in \mathbb{R}^3.$$

Phase space trajectory

Fast modes

Phase space trajectory

1-D manifold

Slow modes

2-D manifold

0-D manifold
(*i.e.* equilibrium point)

R_3

SIM

R_1

R_2

Mathematical Model

For a mixture of mass M confined in volume V containing N species composed of L elements that undergo J reversible reactions,

$$\frac{dn_i}{dt} = V \sum_{j=1}^{J} \nu_{ij} r_j, \quad i = 1, \ldots, N,$$

where,

$$r_j = A_j T^{\beta_j} \exp\left(\frac{-E_j}{\bar{\Re}T}\right) \left(\prod_{i=1}^{N} \left(\frac{n_i}{V}\right)^{\nu'_{ij}} - \frac{1}{K_j^c} \prod_{i=1}^{N} \left(\frac{n_i}{V}\right)^{\nu''_{ij}}\right), \quad j = 1, \ldots, J,$$

$$K_j^c = \left(\frac{p^o}{\bar{\Re}T}\right)^{\sum_{i=1}^{N} \nu_{ij}} \exp\left(-\frac{\sum_{i=1}^{N} \bar{\mu}_i^o \nu_{ij}}{\bar{\Re}T}\right), \quad j = 1, \ldots, J.$$

System reduction

- In chemical reactions, atoms are conserved:

$$\sum_{i=1}^{N} \phi_{li}\nu_{ij} = 0, \qquad l = 1, \ldots, L, \quad j = 1, \ldots, J,$$

$$\sum_{i=1}^{N} \phi_{li}n_i^* = \sum_{i=1}^{N} \phi_{li}n_i, \qquad l = 1, \ldots, L.$$

- Solutions of the following form exist,

$$n_i = n_i^* + M \sum_{k=1}^{R} \mathcal{D}_{ik}z_k, \qquad i = 1, \ldots, N.$$

- The reactive system is recast as an autonomous dynamical system,

$$\frac{dz_k}{dt} = f_k\left(z_1, \ldots, z_R\right), \qquad k = 1, \ldots, R.$$

Method of Construction

Equilibria

- The construction method is based on identifying all the equilibria, and connecting relevant ones via heteroclinic orbits.

- For isothermal reactive systems, reaction rates depend on combinations of polynomials of $\mathbf{z}$.

- The set of equilibria of the full reaction network is complex: $\mathbf{z}^e \in \mathbb{C}^R \mid \mathbf{f}\left(\mathbf{z}^e\right) = \mathbf{0}$.

- This set contains finite and infinite equilibria.

- The system's equilibria can be positive dimensional continua.

SIM construction

- A 1-D SIM has a maximum of two branches that connect two equilibria to the unique physical critical point (a sink) tangent to its slowest mode.

- These equilibria are identified by their special dynamical character: *their eigenvalue spectrum contains only one unstable direction*.

- Heteroclinic orbits are generated tangent to these special equilibria's unstable directions.

- Check first the finite equilibria, then the infinite ones.

Projective space

- One-to-one mapping of the composition space, $\mathbb{R}^R \to \mathbb{R}^R$,

$$Z_k = \frac{1}{z_k}, \quad k \in \{1, \ldots, R\},$$

$$Z_i = \frac{z_i}{z_k}, \quad i \neq k, \quad i = 1, \ldots, R.$$

- This maps equilibria located at infinity into a finite domain.

- To deal with the time singularity, we add the transformation

$$\frac{dt}{d\tau} = (Z_k)^{d-1},$$

where d is the highest polynomial degree of $\mathbf{f}(\mathbf{z})$.

Computational strategy

- We use the `Bertini`[a] software (based on a homotopy continuation numerical technique) to compute the system's equilibria up to any desired accuracy.

- Thermodynamic data is obtained from `Chemkin-II`.

- The SIM heteroclinic orbits are obtained by numerical integration of the species evolution equations using a computationally inexpensive scheme.

- Computation time is typically less than 1 minute on a $2.16\,GHz$ MacBook Pro machine.

[a]D. J. Bates, J. D. Hauenstein, A. J. Sommese, and C. W. Wampler, Bertini: Software for numerical algebraic geometry. Available at: www.nd.edu/∼sommese/bertini.

Zel'dovich Mechanism

- The mechanism consists of $J = 2$ bimolecular reversible reactions involving $N = 5$ species $\{NO, N, O, O_2, N_2\}$ and $L = 2$ elements $\{N, O\}$.

- $\mathbf{z} \in \mathbb{R}^2$, so selected species are $i = \{1, 2\} = \{NO, N\}$.

- The kinetic data are adopted from Baulch *et al.*[b]

- The system is spatially homogenous with isothermal and isochoric conditions, $T = 4000\ K, V = 10^3\ cm^3$.

- Initial number of moles of all species are $\mathbf{n}^* = 10^{-3}\ mol$.

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[b]D. L. Baulch *et al.*, *J. Phys. Chem. Ref. Data*, **34**, pp. 757-1326, 2005.

Reactive system evolution
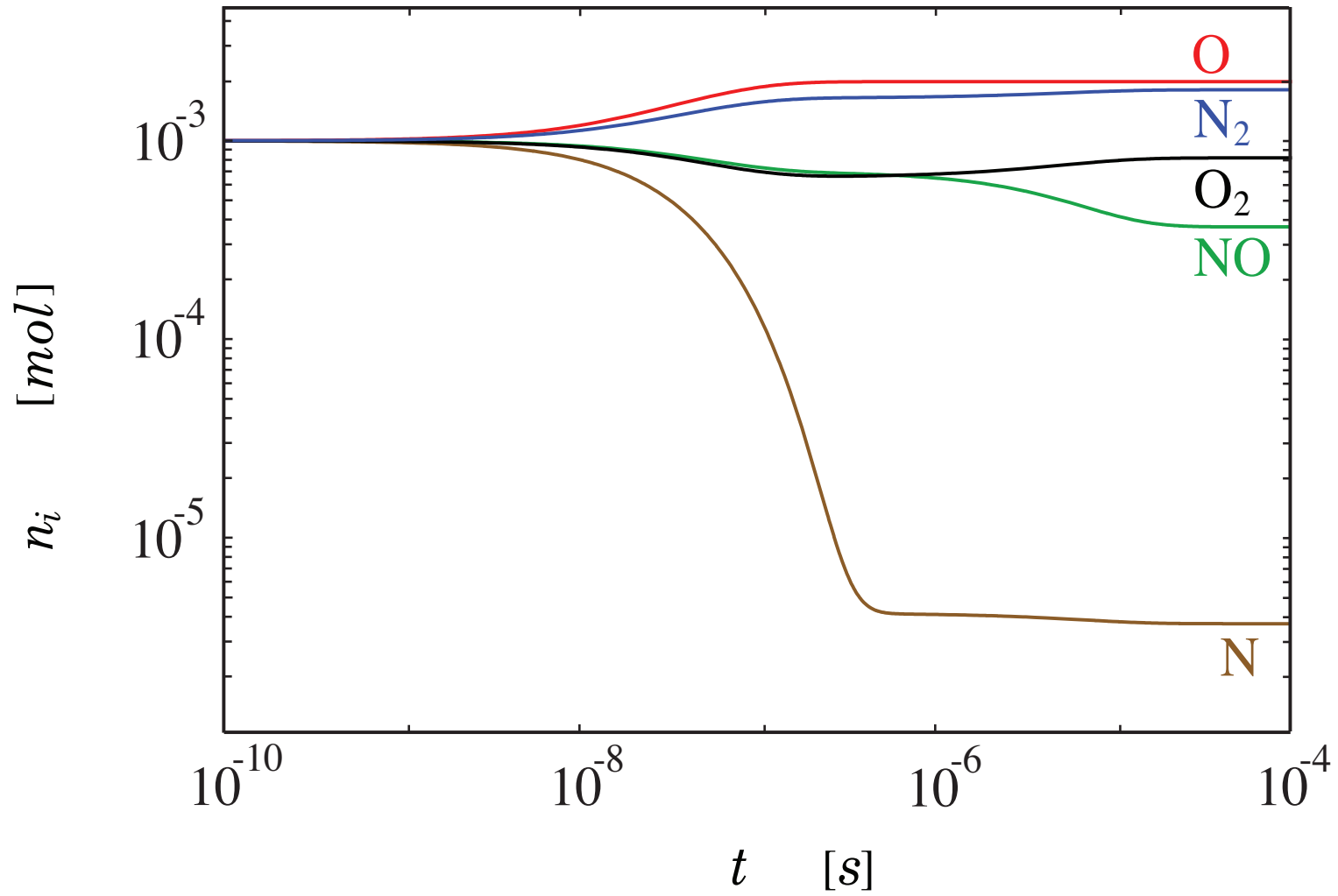
Dynamical system formulation

- The evolution of the system is described by:

$$\frac{d}{dt}\left(\begin{array}{c} z_1 \\ z_2 \end{array}\right) = \left(\begin{array}{c} 2.51 \times 10^2 + 1.16 \times 10^7 z_2 + 6.99 \times 10^8 z_2^2 \\ -9.98 \times 10^4 z_1 - 3.22 \times 10^9 z_2 z_1 \\ 2.51 \times 10^2 - 1.17 \times 10^7 z_2 - 6.98 \times 10^8 z_2^2 \\ +8.47 \times 10^4 z_1 - 1.84 \times 10^9 z_2 z_1 \end{array}\right) \equiv \mathbf{f}(\mathbf{z}).$$

- Employ the projective space mapping with $d = 2$ and $k = 1$:

$$\frac{d}{d\tau}\left(\begin{array}{c} t \\ Z_1 \\ Z_2 \end{array}\right) = Z_1^2 \cdot \left(\begin{array}{c} Z_1^{-1} \\ -Z_1 \, f_1\,(Z_1, Z_2) \\ f_2\,(Z_1, Z_2) - Z_2 \, f_1\,(Z_1, Z_2) \end{array}\right) \equiv \mathbf{F}(\mathbf{Z}),$$
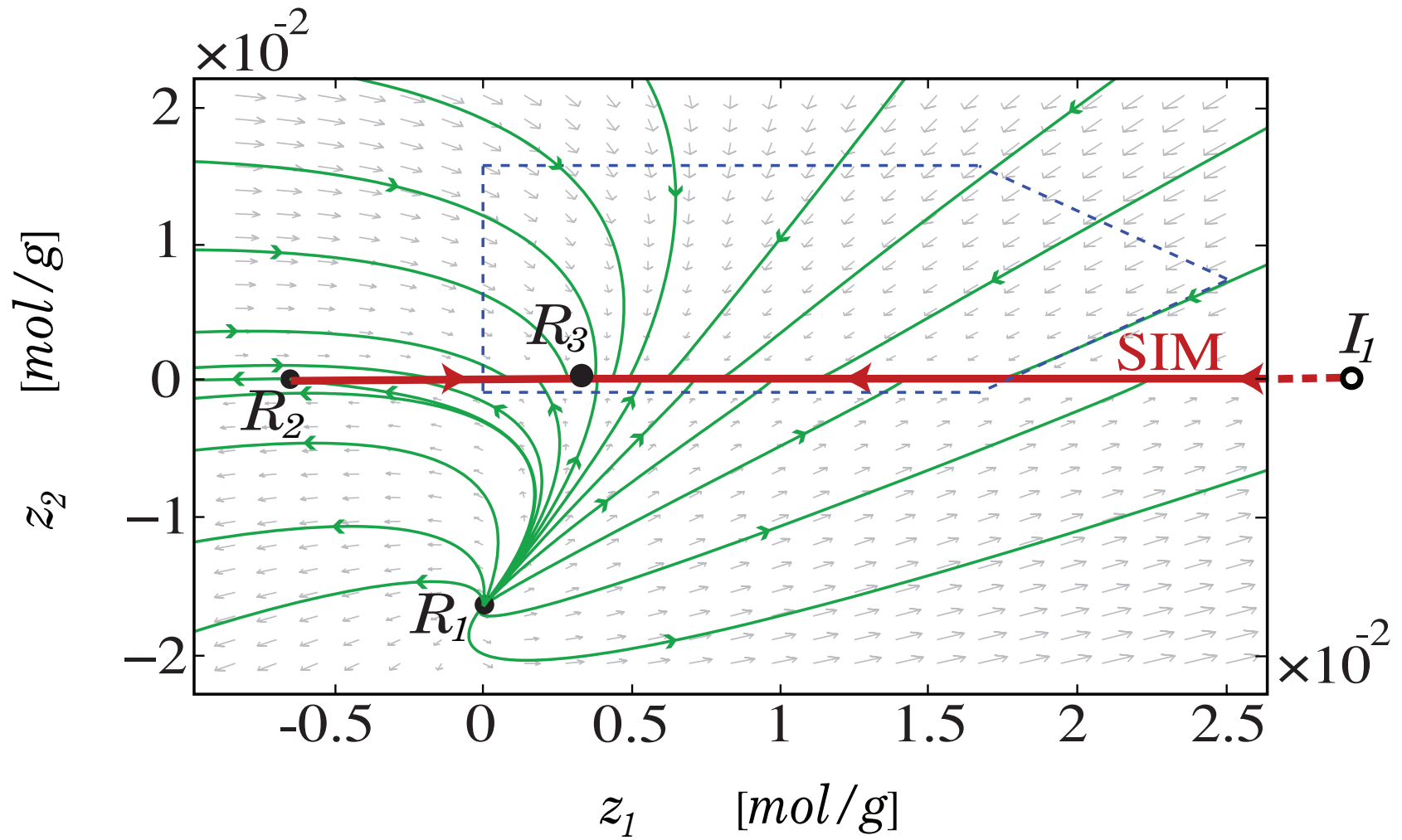
System's equilibria

finite

$$R_1 \equiv (\mathbf{z}^e) = \left(-1.78 \times 10^{-5}, -1.67 \times 10^{-2}\right) \ mol/g,$$
$$(\boldsymbol{\lambda}) = \left(4.18 \times 10^7, 2.35 \times 10^7\right) \ 1/s,$$
$$R_2 \equiv (\mathbf{z}^e) = \left(-4.20 \times 10^{-3}, -2.66 \times 10^{-5}\right) \ mol/g,$$
$$(\boldsymbol{\lambda}) = \left(-4.64 \times 10^6, 7.11 \times 10^5\right) \ 1/s,$$
$$R_3 \equiv (\mathbf{z}^e) = \left(3.05 \times 10^{-3}, 2.94 \times 10^{-5}\right) \ mol/g,$$
$$(\boldsymbol{\lambda}) = \left(-1.73 \times 10^7, -1.91 \times 10^5\right) \ 1/s.$$

infinite

$$I_1 \equiv (\mathbf{Z}^e) = (0,0),$$
$$(\boldsymbol{\lambda}) = \left(-1.84 \times 10^9, 0\right) \ g/mol/s^2,$$
$$I_2 \equiv (\mathbf{Z}^e) = (0, 1.01),$$
$$(\boldsymbol{\lambda}) = \left(2.54 \times 10^9, 1.12 \times 10^9\right) \ g/mol/s^2,$$
$$I_3 \equiv (\mathbf{Z}^e) = (0, 2.60),$$
$$(\boldsymbol{\lambda}) = \left(3.65 \times 10^9, -2.90 \times 10^9\right) \ g/mol/s^2.$$

The system's 1-D SIM

Detailed Hydrogen-Air Mechanism

- Mechanism: $J = 19$ reversible reactions involving $N = 9$ species and $L = 3$ elements. $R = 6$, so that $\mathbf{z} \in \mathbb{R}^6$.

- Kinetic model from Miller *et al.*[c]

- Closed and spatially homogenous system with isothermal and isochoric conditions at $T = 1500\ K$, and $V = 10^{-3}\ cm^3$.

- Stoichiometric mixture $2H_2 + (O_2 + 3.76N_2)$.

- Selected species:

$$i = \{1, 2, 3, 4, 5, 6\} = \{H_2, O_2, H, O, OH, H_2O\}.$$

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[c]J. A. Miller, R. E. Mitchell, M. D. Smooke, and R. J. Kee, *Proc. Combust. Ins.* **19**, pp. 181-196, 1982.

Reactive system evolution

Figure axes: n_i $[mol]$ versus t $[s]$

Labeled curves: O_2, H_2O, H_2, H, OH, HO_2, O, H_2O_2
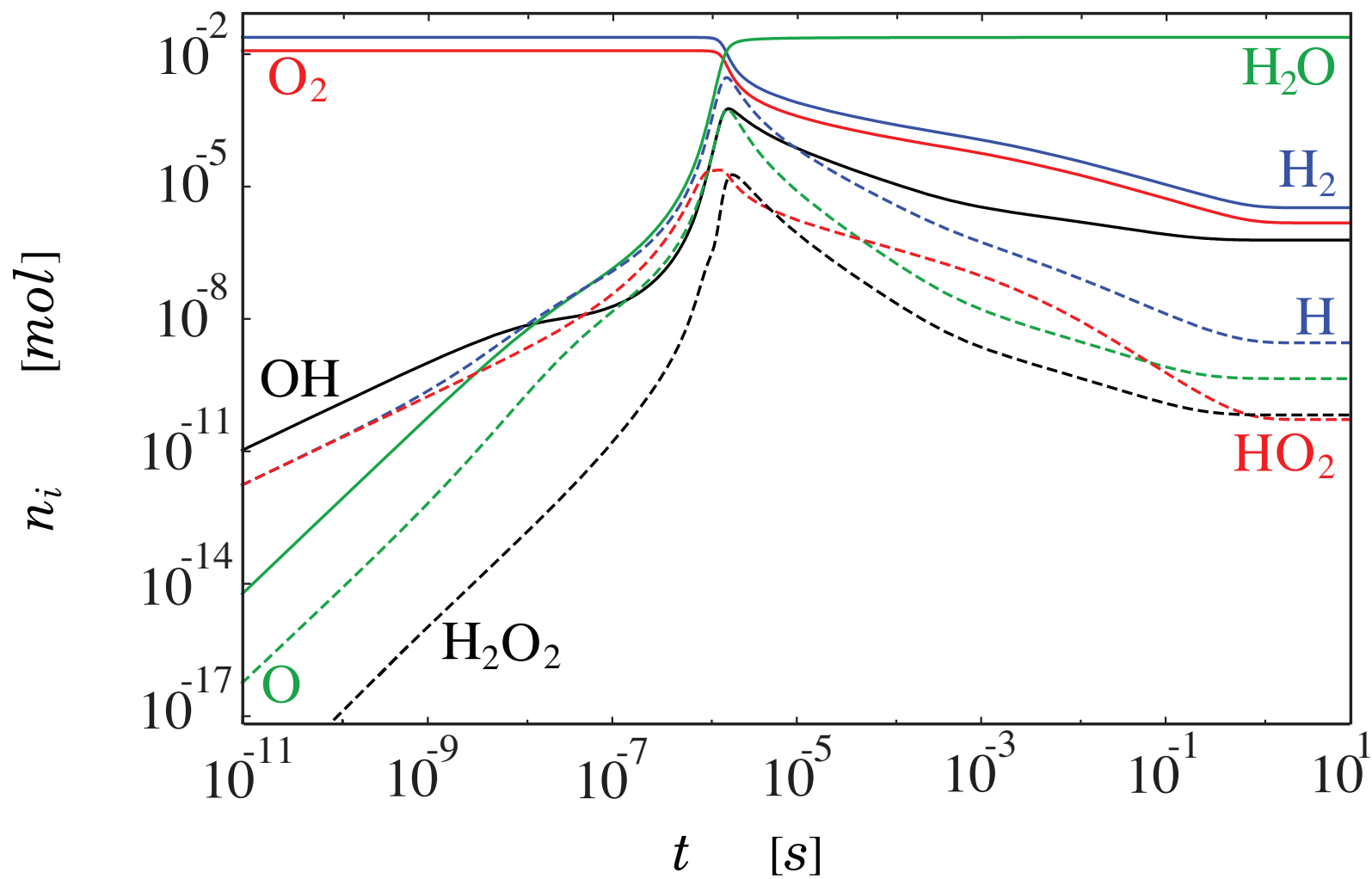
System's equilibria

- The system has 284 finite and 42 infinite equilibria.

- The set of finite equilibria contains 90 real and 186 complex $0\text{-}D$, one $1\text{-}D$, one $2\text{-}D$, and six $3\text{-}D$ equilibria.

- The set of infinite equilibria contains 18 real and 18 complex $0\text{-}D$, and six $1\text{-}D$ equilibria.

- Only 14 critical points have an eigenvalue spectrum that contains only one unstable mode.

- Inside the physical domain there is a unique equilibrium:

$$R_{19} = \left(1.98 \times 10^{-6}, 9.00 \times 10^{-7}, 1.72 \times 10^{-9},\right.$$

$$\left. 2.67 \times 10^{-10}, 3.66 \times 10^{-7}, 1.44 \times 10^{-2}\right) \; mol/g.$$

3-D projection of the system's SIM
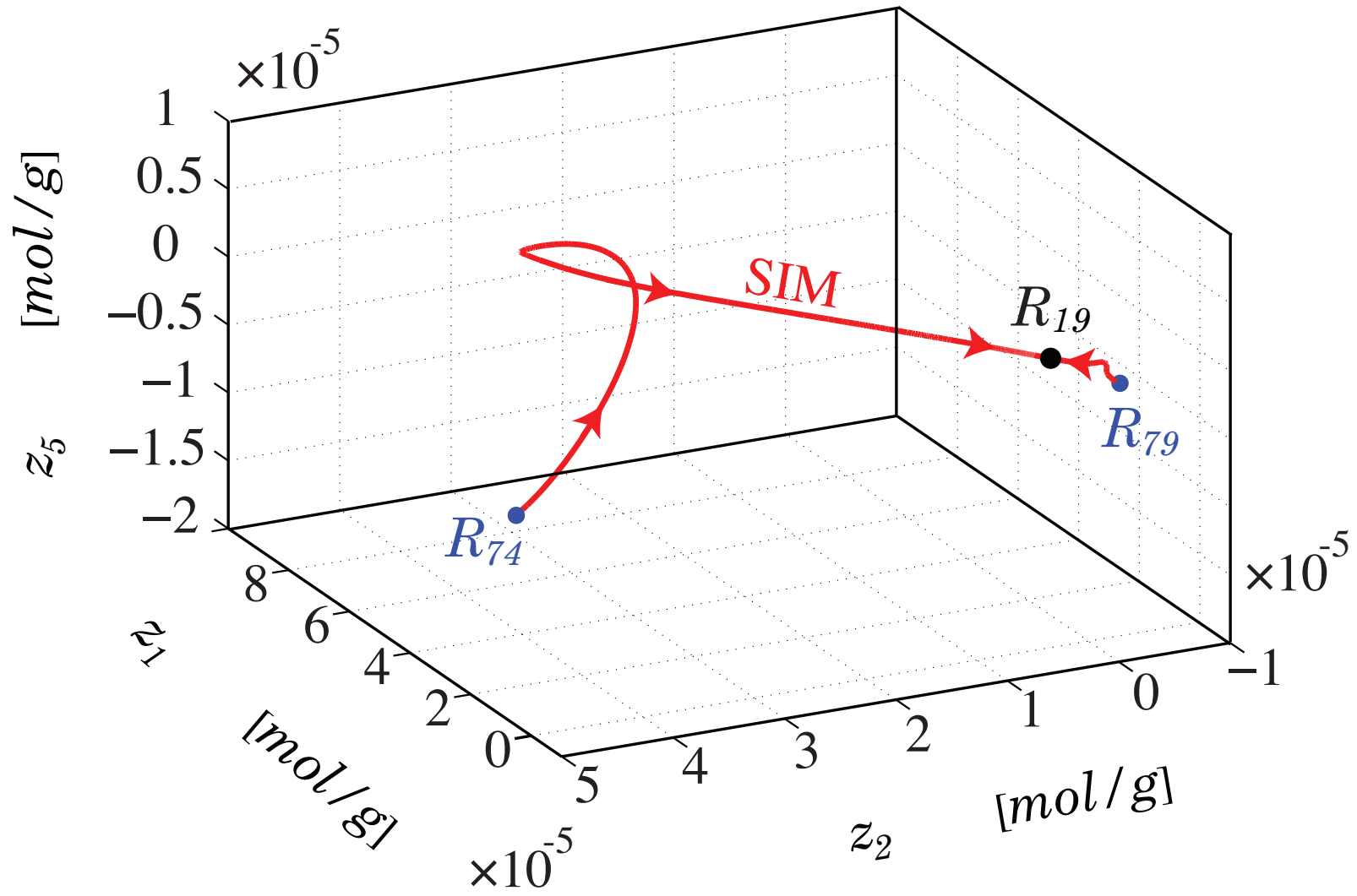
Summary and Conclusions

- Once the difficult task of identifying all equilbria is complete, constructing the actual SIM is computationally efficient and algorithmically easy; thus, there is no need to identify it only approximately.

- Identifying all critical points, finite and infinite, plays a major role in the construction of the SIM.

- The construction procedure can be systematically extended to construct higher-dimensional SIMs.